

THE BOSE GAS LOW MOMENTUM LIMIT REVISITED

H. Perez Rojas^{1,2} and D. Oliva²

¹*International Center for Theoretical Physics,
P.O. Box 586 34100 Trieste, Italy*
²*Grupo de Física Teórica, ICIMAF,
Calle E No. 309, Vedado, La Habana, Cuba.*

We discuss the standard approach to the problem of the low momentum limit of the spectrum for a weakly interacting Bose gas. The Bogoliubovs spectrum is shown to be obtained as a Goldstone mode thanks to the introduction of a chemical potential μ . This procedure has, however, difficulties since the breaking of the gauge symmetry implies that the corresponding chemical potential must be taken as zero, unless it is introduced before breaking the symmetry. But if this is done, after the symmetry breaking μ loses its meaning as a chemical potential. An alternative two-mode solution is suggested having two modes, one of them being the free-particle quadratic in momentum spectrum, the second bearing a gap. This gap leads to a λ -type behavior of the specific heat near the critical temperature.

PACS 05.30.Jp

I. INTRODUCTION

Most studies for the weakly interacting Bose gas deal with the zero temperature approximation. We must cite at first the famous Bogoliubov model [1]. In it the assumption $N - n_0 = \sum_{\mathbf{p}} n_{\mathbf{p}} \ll N$ is made, so that one can discard a term of order $(\sum_{\mathbf{p}} n_{\mathbf{p}})^2$. This leads to a gapless spectrum, but such approximation is actually valid for temperatures extremely close to $0^\circ K$. Bogoliubov's spectrum is in agreement with the pure phenomenological predictions made by Landau concerning the superfluid spectrum, [2] whose lower branch is expected to have a phonon behavior. Far from $0^\circ K$, as happens near and below the critical temperature T_c , the approximation made by Bogoliubov is, however, not valid, and the spectrum bears a gap [3], since it is,

$$\epsilon(p) = \sqrt{(p^2/2m)^2 + 8K(p^2/2m) + 12K^2}, \quad (1)$$

where $K = U_0 n_0 / 2V$, and U_0 is the (approximately) constant potential, n_0 the condensate and V the volume. As shown in [3], this gap, not being satisfactory with the expected spectrum, bears however the interesting property of leading to a divergent behavior of the heat capacity of the system, which fact is in correspondence with the well-known lambda-type phase transition of He^4 . The usual Bogoliubov gapless spectrum does not predict any λ behavior [4] and is valid only near $T = 0$, also it does not exhibit even the discontinuity in the C_v derivative at T_c typical of the usual ideal Bose gas.

Bogoliubov's work was a brilliant insight in the appearance of gapless particles after spontaneous breaking of a gauge symmetry, a fact which became more clear 15 years later, after the Goldstone theorem [15]. After Bogoliubov the weakly interacting gas spectrum was investigated by Beliaev [5], by using the Green's function method, but the correspondence with Bogoliubov's results could be obtained only after introducing a quantity identified as a chemical potential, which was not taken into account in the original model by Bogoliubov. Below we shall see, by a different method than the one used by Beliaev, that spontaneous symmetry breaking is produced by introducing explicitly the chemical potential, leading to the appearance of a gapless Goldstone mode. On the other hand, by taking the chemical potential as equal to zero in Beliaev's calculations, the spectrum (1) is reproduced.

In the present letter we are interested essentially in discussing the meaning of taking such a chemical potential as different from zero, at the light of the fundamental principles of statistical mechanics.

II. THE HAMILTONIAN

Condensation breaks the gauge symmetry (see below). The introduction of a chemical potential coupled to a Noether charge Q associated to a broken symmetry in the density matrix was investigated in the relativistic context in papers [8]. Such charge has many odd features from which we mention two: first, in general, it is not conserved, and second, its introduction ban the fulfillment of the Kubo-Martin-Schwinger (KMS) condition required for the statistical description of systems in thermodynamical equilibrium, since according to the Araki-Haag-Kastler-Takesaki (AHKT) theorem [9], only those charges that belong to the center of the unbroken part of the symmetry group satisfy the KMS condition and can have a chemical potential associated to them.

In the non-relativistic weakly interacting Bose gas case, the charge operator associated to the broken symmetry is $N = \int d^3x \psi^*(x)\psi(x) = \sum_{p=0}^{p \rightarrow \infty} a^*(p)a(p)$, where it is taken the condensate density as $a^*(0)a(0) = n_0$ and in consequence $a(0) = \sqrt{n_0}e^{i\theta}$, $a^*(0) = \sqrt{n_0}e^{-i\theta}$. This means [10] that the physically relevant representations of the algebra of canonical variables are labelled by the parameters n_0, θ , and

$$\lim_{V \rightarrow \infty} \int d^3x \langle n_0, \theta | \psi(x) | n_0, \theta \rangle = \sqrt{n_0} e^{i\theta} \quad (2)$$

which for $n_0 \neq 0$ is not invariant under gauge transformations

Let us consider the Lagrangian

$$\mathcal{L} = -\psi^*(x)i\partial_0\psi(x) + \psi^*(x)\frac{\nabla^2}{2m}\psi(x) - \lambda(\psi^*(x)\psi(x))^2 \quad (3)$$

where $\lambda = \frac{U_0}{2V}$ and we are considering the approximation of a constant repulsive potential. Under the gauge transformation

$$\psi(x) \rightarrow e^{i\alpha}\psi(x) \quad (4)$$

terms having equal number of $\psi(x)$ and $\psi^*(x)$ are gauge invariant, so \mathcal{L} is gauge invariant, as it is also the density of particles N .

From the Lagrangian we can get immediately the Hamiltonian in which, by taking the Schrodinger representation of the fields $\psi(x) = \frac{1}{V} \sum a(p)e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$, $\psi^*(x) = \frac{1}{V} \sum a^*(p)e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}$, one obtains in momentum space an expression quadratic in the fields $a^*(p)$, $a(p)$. After condensation, if it is taken $a^*(p) = a^*(p)e^{-i\theta}$ and $a(p) = a(p)e^{i\theta}$ obviously, such a Hamiltonian is not gauge invariant. If we fix the gauge $\theta = 0$, we get finally the bilinear part of the Bogoliubov's Hamiltonian,

$$H_B = \lambda n_0^2 + \sum_p [a^*(p)\frac{p^2}{2m}a(p) + K(4a^*(p)a(p) + a^*(p)a^*(-p) + a(p)a(-p))] \quad (5)$$

where $K = \lambda n_0$. Note that the coefficient of the first "potential" term is $4K$ and *not* $2K$, as is done as an approximation in the usual treatment of the problem in terms of the total number of particles N .

III. DENSITY MATRIX AND BELIAEV EQUATIONS

The immediate task is to build a density matrix aimed to obtain the partition functional \mathcal{Z} . If we name $N_p = \sum_p a^*(p)a(p)$ the operator for the number of excited particles, we see that $[H_B, N_p] \neq 0$. In consequence, there is no a common set of eigenstates for these two operators and the density matrix $\rho = e^{-(H_B - \mu N_p)\beta}$ is an ill-defined one for describing states of equilibrium. If we define $\Omega = -\beta^{-1} \ln \mathcal{Z}$ one cannot state that $N = -\frac{\partial \Omega_\beta}{\partial \mu}$, is the average number of excited particles. However, one might argue that we have the right to consider $\mu \neq 0$ as a Lagrange multiplier, since in building ρ and Ω it loss the meaning of a chemical potential but then we face new difficulties.

Working according to Bogoliubov's standard procedure [2], we may proceed to diagonalize H_B ,

$$H_B = \sum_{\mathbf{p}} \epsilon(p) b^*(p) b(p) \quad (6)$$

where according to Bogoliubov's transformation, we have $b^*(p) = [a(p) + \alpha_p a^*(-p)]/(1 - \alpha^2(p))$, $b(p) = [a^*(p) + \alpha_p a(-p)]/(1 - \alpha^2(p))$, and $\alpha(p) = [4K + p^2/2m - \epsilon(p)]/2K$. In this representation, in which $b^*(p)b(p)$ is gauge

invariant under the transformation $b(p) \rightarrow e^{i\theta}b(p)$, $b^*(p) \rightarrow e^{-i\theta}b^*(p)$, we have

$$N = \sum_p \frac{(1 + \alpha(p)^2)n_p + \alpha(p)^2}{1 - \alpha(p)^2} - \frac{\alpha_p}{1 - \alpha(p)^2} (b^*(p)b^*(-p) + b(p)b(-p)), \quad (7)$$

which is obviously not gauge invariant. The conditions of the AHKT theorem [9] are not satisfied. Thus, the system of equations (17) and (18) are also not gauge invariant.

Thus if we continue in a pure formal way, and leave $\mu \neq 0$, by considering $H_B - \mu(N_p + n_0)$ as a new Hamiltonian, one can obtain some partition function \mathcal{Z} from it, from which the system of Green functions and the thermodynamical potential Ω can be obtained. By introducing adequate external sources, we have for the partition function obtained from the unperturbed Hamiltonian H_B ,

$$\mathcal{Z}(\eta, \zeta) = M(\beta) e^{-\beta V \lambda n_0^2 - \mu n_0} \mathcal{Z}_\beta \quad (8)$$

where $M(\beta)$ is a temperature dependent constant and

$$\mathcal{Z}_\beta = \int \mathcal{D}a^* \mathcal{D}a e^{\sum_{p_4, p} [S(p) + \eta(p)a^*(p) + \zeta(p)a(p)]} \quad (9)$$

and

$$S(p) = (ip_4 + \mu - \frac{p^2}{2m})a^*(p)a(p) - K(4a^*(p)a(p) + a^*(p)a^*(-p) + a(p)a(-p)) \quad (10)$$

We may consider the interaction term in the Hamiltonian, containing terms of third and fourth order in $a^*(p), a(p)$. If $V(a(0), a^*(0), a^*(p), a(p))$ is such term, the interacting partition function is $\mathcal{Z}_I = e^{\sum_{p_4, p} V(a(0), a^*(0), \frac{\delta}{\delta \eta(p)}, \frac{\delta}{\delta \zeta(p)})} \mathcal{Z}$. By using the standard methods of functional differentiation, we may develop a formalism to obtain from \mathcal{Z}_I the equations for the Green functions $G(p, p') = \delta^2 \mathcal{Z}_I / \delta \zeta(p) \delta \eta(p')$, $G_1(p, p') = \delta^2 \mathcal{Z}_I / \delta \eta(-p) \delta \eta(p')$. We will restrict, however, to the corresponding expressions for the $V = 0$ approximation $\mathcal{Z}_I = \mathcal{Z}$, by taking the bilinear terms in (10), and by calling $G_0^{-1} = (ip_4 + \mu - \frac{p^2}{2m})$ one easily gets,

$$G(p) = G_0(p) + 4KG_0(p)G(p) + 2KG_0(p)G_1(p) \quad (11)$$

$$G_1(p) = 2KG_0(-p)G(p) + 4KG_0(-p)G_1(p) \quad (12)$$

These are a simplified version of the Beliaev's equations [5], which lead to

$$G_1(p) = \frac{2KG(p)}{G_0^{-1}(-p) - 4K} \quad (13)$$

$$G(p) = \frac{G_0(-p) - 4K}{(p_4 - i\epsilon(p))(p_4 + i\epsilon(p))} \quad (14)$$

where

$$\epsilon(p) = \sqrt{(\frac{p^2}{2m} - \mu + 4K)^2 - 4K^2}. \quad (15)$$

The effective potential is obtained as $U = \beta^{-1} \ln \mathcal{Z}/V$, by defining $\xi = \sqrt{n_0}$, as

$$U = \lambda \xi^4 - \mu \xi^2 + \Omega_\beta \quad (16)$$

where $\Omega_\beta = \ln \mathcal{Z}_\beta$. We see that the chemical potential μ plays an essential role in showing explicitly the symmetry breaking term in U , analogous to the "negative mass term" of the usual relativistic theory [15]. Its presence leads necessarily to the existence of Goldstone bosons.

From (16) one can obtain the condition of extremum of U ,

$$\frac{\partial U}{\partial \xi} = 4\lambda\xi^3 - 2\mu\xi + \frac{\partial \Omega_\beta}{\partial \xi} = 0, \quad (17)$$

But we cannot write that the quantity

$$-\frac{\partial U}{\partial \mu} = n_0 + \frac{\partial \Omega_\beta}{\partial \mu} \quad (18)$$

as the average number of particles, i.e, $N_q = -\frac{\partial \Omega_\beta}{\partial \mu}$ is not the number of excited particles. Usually it is interpreted as the average number of "quasiparticles". For $T \rightarrow 0, N_q \rightarrow 0$ and only in that case $n_0 \sim N$.

The equation (17) gives $\xi^2 = \mu/2\lambda$ as the minimum at the tree level, i.e., for $T = 0$ $\mu = 2K$. By substituting in (15), this leads immediately to the (gapless) Goldstone boson $\epsilon(p)_B = \sqrt{(\frac{p^2}{2m})^2 + 4K\frac{p^2}{2m}}$, which is the usual Bogoliubov spectrum. According to Goldstone theorem, these modes if calculated correctly, would maintain gapless at all orders of perturbation theory. This result is in correspondence to the one obtained, before the formulation of the Goldstone theorem, by Hugenholtz and Pines [11].

We see that for the reasons pointed out above, there is no right to build a density matrix in the grand canonical ensemble by subtracting from H_B the operator N_p multiplied by a nonzero chemical potential μ , since as $[H_B, N_p] \neq 0$, there is no a common set of eigenstates and eigenvalues for them, and $\rho = e^{-(H_B - \mu N_p)\beta}$ does not satisfy the KMS condition. Thus, it is unsatisfactory to attribute a standard physical meaning to quantities derived from it if $\mu \neq 0$, in particular, to interpret $\frac{\partial \Omega_\beta}{\partial \mu}$ in (18) as the average number of excited particles. We introduce the notion of "quasiparticles" in part to avoid such a difficulty. We point out also that if we take $\mu = 0$ (15) turns into (1).

IV. ALTERNATIVE PROCEDURE

We conclude that the standard introduction of a chemical potential is not satisfactory if it is done after breaking the gauge symmetry. If we include it before the symmetry breaking, it loss its meaning as a chemical potential and becomes a parameter essential for the fulfillment of the Goldstone theorem. However it leads (according to the gauge fixing) to other infinite non-equivalent set of representations of the operator algebra, and of their dynamics [10]. There is no a priori criteria to state which of these representations is physically better. One may choose, for instance, that one wants the energy eigenvalue $E(p)$ to be linear in p for $p \rightarrow 0$. Then one possible solution is the Bogoliubov-Beliaev spectrum. But from the point of view of Goldstone theorem and its consequences, the use of the fields $\psi^*(x)$ and $\psi(x)$, both containing the symmetry-breaking parameter, is rather obscure. Only one physical mode is present. It would ban the appearance of a pure gapless mode and a mode bearing a gap, which is to be expected (from the Goldstone theorem point of view) since we are using two-component fields.

If we do not tie to the linear mode requirement, an alternative model is, for instance, the one obtained by taking in (3) $\psi = \xi + \sigma(x) + i h(x)$. At the tree level these two modes have the spectra $E_h = p^2/m$ and $E_\sigma = p^2/m + \Delta_\sigma$ where $\Delta_\sigma = K = \lambda n_0$ and n_0 is the condensate (which is the total number of particles at $T = 0$) The first mode has the property of being gapless, and trivially corresponds to the Goldstone Boson [15], since $E_h \rightarrow 0$ for $p \rightarrow 0$. The second mode bears a gap. At $T \neq 0$, this gap is expected to be of form $\Delta_\sigma(T) = \lambda n_0 \sqrt{1 - (\frac{T}{T_c})^3}$, where T_c is the critical temperature for condensation. It bears the interesting property of leading to a λ -behavior near T_c , as shown below. We observe that the Bogoliubov-Beliaev spectrum is just the geometric average of the spectra $E(p) = \sqrt{E_\sigma E_h}$ this spectrum does not lead to an λ -type behavior.

The divergence of the specific heat c_V is seen [3] easily starting from E_σ . One can write the thermodynamic potential as $\Omega = AT \int_0^\infty p^2 dp \ln(1 - e^{-\epsilon_n \beta})$, where A is a constant. By taking $x = p/\sqrt{2mT}$, in the infrared limit, where p_0 is a sufficiently small momentum, we have

$$\Omega \sim -\frac{A}{3} \int_0^{p_0} \frac{p^4 dp}{m(e^{\epsilon_n \beta} - 1)} \sim -\frac{A(2mT)^{5/2}}{3m} \int_0^{p_0} \frac{x^4 dx}{x^2 + \Delta_\sigma T^{-1}} \sim -\frac{A(2m)^{3/2} T \Delta_\sigma^{3/2} \pi}{6}. \quad (19)$$

From $c_V = -T \frac{\partial^2 \Omega}{\partial T^2}$, we get that c_V diverges as $\Delta_\sigma^{-1/2}$ for $T \rightarrow T_c$.

It may be argued however, that the existence of a gap, as well as the non-linear gapless mode, contradicts the generally accepted idea of a phenomenological linear in p phonon spectrum [2]. One concludes that the model we are considering is an oversimplification of the real system, and that one must study the higher order corrections. Work in this sense is in progress. Another modification would be to introduce some term accounting for the oscillatory

motion of the condensed or quasi-condensed atoms (the spectra obtained above refers actually to translational modes), leading to a phonon field having linear behavior of the spectrum. New models for superfluidity are currently being elaborated [14] on much more phenomenological basis by including such vibrational terms.

Acknowledgements

The work have been supported by *Ministerio de Ciencia Tecnología y Medio Ambiente* under the grant CB0407. The authors would like to thanks the invitation and hospitality of the Abdus Salam International Center for Theoretical Physics ICTP and in particular to Prof V. Kravtsov, Head of the Condensed Matter Section, allowing the visit to the Center of one of the author (D.O.A).

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